Diesel Engine Combustion Simulation using Computational Fluid Dynamics

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***Abstract*- Diesel engines are used in automotive and stationary applications. The main problem with diesel engines is emissions of nitrogen oxides (NOx) and particulates. In order to minimize the emissions, it is necessary to design the diesel engine with better in-cylinder flow (air-fuel mixing) and combustion process. Computational Fluid Dynamics (CFD) simulation helps to understand the Diesel engine temperature distribution and NOx species concentrations with respect to time. A small direct injection (DI) engine was chosen for the study. CFD simulation results were compared with that of engine emission tests. Results were found to be in agreement with NOx emissions. This paper also presents the simulation results of direct injection diesel engine in-cylinder flow (air-fuel mixing) and combustion.**

***Index Terms* - CFD, Diesel engine, combustion modeling**

I. INTRODUCTION

Direct - injection diesel engines are used both in heavy-duty applications and light duty ones due to their high thermal efficiency and low CO_2 emissions [1]. Fuel economy and emission norms are compelling to develop more efficient and cleaner engines. It is necessary to improve the combustion process to reduce exhaust emissions. Computational Fluid Dynamics is popularly used in different stages of engine design and optimization. The combustion system performance can be better understood using CFD simulation. The challenge in using CFD is the complexity of interaction of flow, turbulence, spray and combustion inside the IC engine cylinder. High-pressure injection [2-5] and modification of combustion chamber geometry [6-9] were tried to reduce particulate emissions. Exhaust gas recirculation (EGR) [10] is another technique used to reduce NOx emissions. Supercharging coupled with better injection timing reduces PM emission and NOx reduction [11]. These methods however, have a trade-off relationship between NOx and particulate emissions. To optimize the combustion and emissions in diesel engine it is necessary to understand the flow inside the cylinder. This paper presents the CFD simulation of a diesel engine combustion process to predict the temperature distribution inside the cylinder and NOx emission with reference to crank angle variation in the expansion stroke.

II. ENGINE PARAMETERS

The specifications of the engine are given in Table I. The physical modeling of the injector was not used since preset models of fuel injectors were available in the software used for analysis. The motion of valves also cannot be included in the simulation.

TABLE I.
ENGINE SPECIFICATIONS

Model No	4360
Bore (mm)	82
Stroke (mm)	68
Displacement (cm^3)	359
Comprssion ratio	18:1
RPM	3600
HP	7.5

III. COMPUTATIONAL DOMAIN

The 3-Dimensional model shown in figure 1 is used for the analysis. The simulated engine has a direct injected diesel one with 4 - hole injector and eccentric bowl combustion chamber. For numerical integration the structured (hexahedral) mesh is used. During the solution, as the piston moves, the internal mesh structure deforms automatically to minimise the distortion of each individual cell. Figure 1 and 3 shows the geometry and mesh distribution when piston at a bottom dead center (BDC) and the injection parameters are given in Table II.

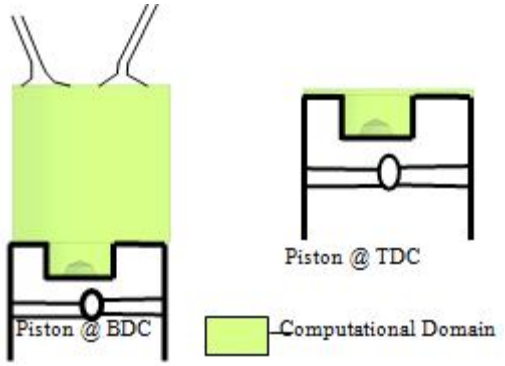

Figure 1. Computational model of the Combustion chamber.

The starting Crank angle when piston @ BDC is 180^0. For each stroke corresponding crank angle is 180^0, total for 4 stroke 720^0 CA). Injection starts @ 343^0 CA means, when piston moves from BDC to TDC, the fuel injection starts 17^0 CA before TDC. Total injection duration 24^0 CA means fuel injection starts 17^0 CA before TDC and ends with 7^0 after TDC). Figure 2 shows the piston movement profiles.

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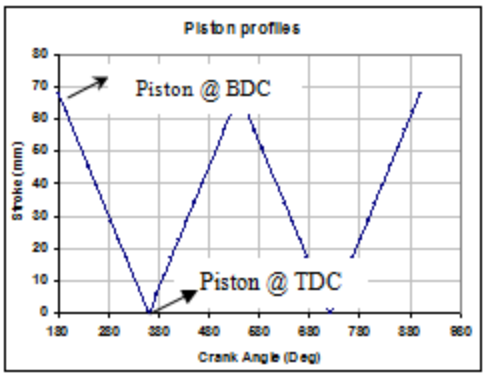

Figure 2. Piston movement profiles.

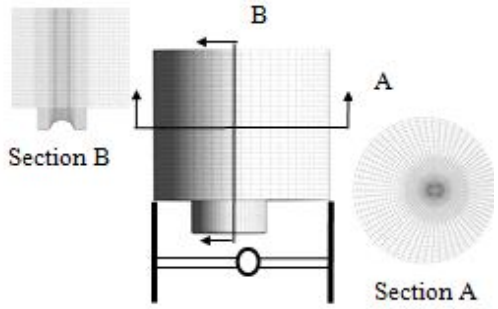

Figure 3. Computational mesh of the Combustion chamber.

TABLE II.
INJECTION PARAMETERS

Type	Direct injection with single central injector
Number of nozzles	4
Total flow rate (g/cycle)	0.05
Start time (CA)0	343
Stop time (CA)0	367
Mean diameter (m)	1 e-06

IV. METHOD USED FOR ANALYSIS OF SIMULATION DATA

The numerical simulations in this investigation are performed based on the commercial computational fluid dynamics software. The various models used in the analysis to represent complex processes are explained below.

A. Turbulent In-cylinder Flow Modeling

In a DI Diesel engine, the fuel is sprayed directly into the cylinder through the fuel injection nozzle. The fuel is then broken into a number of droplets. These droplets undergo collision and coalescence processes, exchanging momentum and energy with the high temperature and pressure surrounding gases inside the cylinder. Finally the droplets evaporate into vapor and mix with air. The equations governing the in-cylinder flow are species transport equations, continuity equation, momentum equation, energy equation, gas state equation and turbulence equations.

Species Transport Equation:

$$\frac{\partial \rho_m}{\partial t} + \nabla.\left(\rho_m \vec{u}\right) = \nabla.\left[\rho D \nabla\left(\frac{\rho_m}{\rho}\right)\right] + \rho_m^c + \rho^s \qquad (1)$$

The last two terms on the right hand side of Eqn.(1) are the source terms due to the chemical reaction and fuel spray, respectively.

Overall Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \nabla.\left(\rho \vec{u}\right) = \rho^s \qquad (2)$$

Momentum Equation:

$$\frac{\partial}{\partial t}\left(\rho \vec{u}\right) + \nabla.\left(\rho \vec{u}\vec{u}\right) = -\nabla p - \nabla\left(\frac{2}{3}\rho k\right) + \nabla.\bar{\bar{\sigma}} + \vec{F} + \rho \vec{g} \qquad (3)$$

where $\vec{F}$ is the source term due to the fuel spray.

Energy Equation:

$$\left[\frac{\partial(\rho e)}{\partial t} + \nabla.\left(\rho \vec{u} e\right) = -p\nabla.\vec{u} - \nabla.\left[-k\nabla T - \rho D \sum_m h_m \nabla\left(\frac{\rho_m}{\rho}\right)\right] + \rho\varepsilon + q^c + q^r\right] \qquad (4)$$

The last two terms on the right hand side of Eqn.(4) are the source terms due to the chemical heat release and fuel spray interactions, respectively.

State Equation:

$$P = RT \sum_m \left(\frac{\rho_m}{w_m}\right) \qquad (5)$$

The turbulence effect is accounted by using the standard k-ξ model [1]. In this model, Reynolds stresses are related to the mean flow using the Bousinesq hypothesis. The turbulent kinetic energy k and turbulent dissipation rate ξ are solved through the following transport equations.

$$\frac{\partial \rho k}{\partial t} + \nabla.\left(\rho \vec{u} k\right) = \left[\frac{2}{3}\rho k \nabla.\vec{u}\right] + \sigma : \nabla \vec{u} + \nabla.\left[\left(\frac{\mu}{\rho \gamma_k}\right)\nabla k\right] - \rho\varepsilon + W^s \qquad (6)$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla.\left(\rho \vec{u} \varepsilon\right) = \left[\frac{2}{3}C_{\varepsilon_1} - C_{\varepsilon_2}\right]\rho\varepsilon\nabla.\vec{u} + \nabla.\left[\left(\frac{\mu}{\rho \gamma_\varepsilon}\right)\nabla\varepsilon\right] + \frac{\varepsilon}{k}\left[C_{\varepsilon_1}\sigma : \nabla\vec{u} - C_{\varepsilon_2}\rho\varepsilon + C_{\varepsilon_3}W^s\right] \qquad (7)$$

where the values of the constants are given as follows: $C_{\varepsilon 1}$ =1.44, $C_{\varepsilon 2}$ =1.92, $C_{\varepsilon 3}$ = -1.0, Pr_k=1.0, Pr_ε=1.3. W^s is the source term due to interaction of air and fuel spray, which is the negative of the rate at which the turbulent eddies are doing work in dispersing the spray droplets.

As the spray is the dominant feature of the flow with in a diesel engine combustion chamber, accurately resolving the spray atomization is a prerequisite for diesel engine simulation. Two mechanisms used for break up of spray are Kelvin-Helmholtz (K-H) inertia instability and Rayleigh-Taylor (R-T) accelerative instability mechanisms. It is assumed that the mechanism responsible for the break up of the spray are classical fluid dynamic instabilities which act at the interface between two fluids of different densities. For both of the instabilities, the time that the spray droplet breaks up is determined from the growth rate of the fastest growing wavelength predicted by the classical instabilities. For the K-H mechanism, the wavelength of the fastest growing wave is given by Reitz [12]. The R-T break up mechanism [14] is employed to account for the effect of rapid

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deceleration of the drops on the atomization process. The K-H and R-T mechanisms compete to break up the spray. More details of break up mechanisms are described in Ref.[12] and [14].

B. NOx Model

Both Nitric Oxide and Nitrogen dioxide are formed during the combustion process in a diesel engine. Generally speaking, NO_2 concentration is negligible compared with NO concentration. It is usually considered to be a transient intermediate species existing only at flame conditions, and it is subsequently converted back into NO in the post-flame region. Thermal NO formation is the most predominant in a diesel engine among the different NO formations. The most widely accepted simplified thermal NO formation mechanism is the extended Zeldowich-NO [19]. The elementary reactions for this mechanism are:

$$O + N_2 \rightarrow NO + N \quad (8)$$
$$N + O_2 \rightarrow NO + O \quad (9)$$
$$N + OH \rightarrow NO + H \quad (10)$$

Among the three reactions, the reaction (8) has the highest activation energy, due to the strong bond in the N_2-molecule. It is the rate-limiting step of the thermal NO formation, and determines the overall process of the NO formation. The reaction rate coefficients for these reactions are given in Arrhenius form:

$$K_f = AT^{\xi} \exp\left(\frac{-E}{T}\right) m^3/(mol - s) \quad (11)$$

The constants A, ? and E used for this investigation are from Hanson and Salimian, et al., [16]. They are given in Table III.

TABLE III.
CONSTANTS FOR THE KINETIC REACTION COEFFICIENTS.

Equation No	Forward Reaction			Backward Reaction		
	A	ξ	E	A	ξ	E
(8)	3×10^{12}	0	15780	0	0	0

C. Combustion Model

The combustion inside the cylinder is modeled by four kinetic reactions and six equilibrium reactions. The four kinetic reactions include those three elementary reactions for thermal NO and a forward reaction representing the oxidation of the fuel, which is considered to be consisting of $C_{12}H_{26}$ only. The fuel oxidation reaction is given below.

$2\ C_{12}H_{26} + 37O_2 \rightarrow 24CO_2 + 26H_2O$

D. Initial and Boundary conditions

The computation started from the end of intake stroke at the bottom dead center corresponding to 180^0 Crank angle and terminated at the end of expansion stroke corresponding to 540^0 CA. The pressure and temperature of the air inside the chamber on the starting of the analysis were set as 100kPa and 350K based on the values given by Bedford [17] and Strauss [18]. No slip conditions were used on the walls. Standard wall functions were used for turbulence models. The amount of fuel injected was 0.05 g/cycle. The normal operating parameters were :

Injection duration: 24^0 CA; Injection start timing:343^0 CA

V. RESULTS AND DISCUSSION

The engine emission readings measured using gas analyzer and values are given in Table IV.

TABLE IV
GAS ANALYZER READING (AT FULL LOAD CONDITION AND AT 3400 RPM)

CO	[% vol]	3.71
HC hexane	[ppm vol]	4539
CO_2	[% vol]	7.67
NO	[ppm vol]	843

Temperature Distribution at various crank angles:

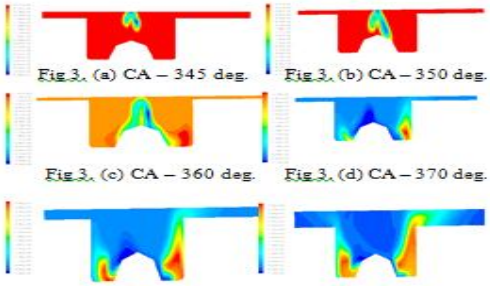

Fig 3. (a) CA – 345 deg. Fig 3. (b) CA – 350 deg.

Fig 3. (c) CA – 360 deg. Fig 3. (d) CA – 370 deg.

Fig 3. (e) CA – 375 deg. Fig 3. (f) CA – 385 deg.

Figure 3(a) to 3(f) presents the in-cylinder temperature distributions from the CFD simulation of base case design. The temperature distributions plotted for different crank angles on a vertical plane. Figure 3(a) shows the maximum temperature of around 950K which is attained from compression stroke. From 343 – 720 crank angle the temperature distribution plotted in Figure 6. Figure 3 (c) shows the initial flame occurs just before compression stroke. The spray and flame reaches the edge of the piston bowl with in short period 7-10 CA deg. The concentration of oxygen in the high temperature zone is very high resulting in a high NOx rate of formation. Figure 4 and 5 shows the NO formation and Soot formation inside the cylinder.

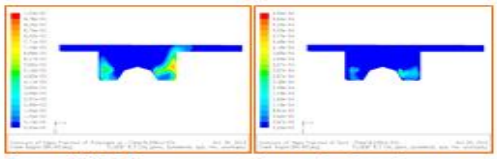

Figure 4. NO formation. Figure 5. Soot formation.

TABLE V

	[ppm vol]
Experiment	843
CFD Simulation	805 – 820 (max)

The NO from emission test is 843 ppm at 3400 rpm. The detailed time history of spray, fuel mass fraction and temperature distributions provided by the CFD simulation are valuable towards gaining a better understanding of the features of combustion for given engine configurations. The temperature distribution inside the cylinder for different crank angles, and NO emissions are given above. NOx formation is highly sensitive to temperature and also effected by species concentration. In-fact the flame in the eccentric

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bowl is not sufficient to burn a complete combustion because of the bowl shape. Table V presents the comparison of simulated and measured emission (NO) for the baseline case. The deviations from experiment and simulation results of NO emission are around 3-5 %. It was found that the general agreement between prediction and engine test was good.

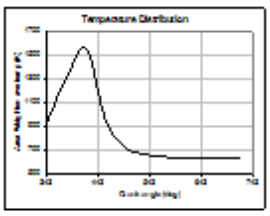

Figure 6. Static temperature.

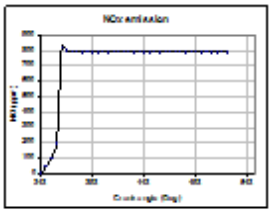

Figure 7. NOx emission.

CONCLUSION

In-cylinder physical variations of a single cylinder diesel engine have been investigated using a CFD simulation code and validated with experimental measurements. Temperature profiles as well as NOx emissions contour from CFD has a good agreement with experimentally measured data. For reducing NOx emission it is no doubt that a precise estimation of flame temperature and a good description of reaction chemistry is essential. The detailed time history of spray, fuel mass fraction and temperature distributions provided by the CFD simulation is valuable towards gaining a better understanding of the feature of combustion.

Since the adopted methodology for the base case has given a high confidence level for further optimization geometry (bowl shapes) and operating parameters (Injection duration, Start of Injection timings) can be carried out for reducing NOx emissions through CFD.

NOMENCLATURE

A = Constant
E = Activation temperature
e = Specific internal energy
F = Rate of momentum gain per unit volume due to the fuel spray
g = Gravity
h_m = Specific enthalpy of species m
q_c = Rate of heat release per unit volume
q_s = Rate of heat gain per unit volume due to spray interactions
R_0 = Universal gas constant
W_m = Molecular weight of species
W_s = Source term due to the interaction of air and fuel spray
ñ = Mass density
$ñ_m$ = Mass density of species m
$ñ_C$ = Rate of mass gain per unit volume from chemical reactions
$ñ_s$ = Rate of mass gain per unit volume from fuel spray
K_r = Reaction rate coefficient
ó = Viscous stress tensor
µ = Viscosity
î = Constant
D = Diffusion CoefficientA.

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